

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 178 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.44e-01

Confidence level: 7.23e-01

Nearest Neighbors from the Training Set

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Butylbenzene

Measured: 2450

Predicted: 1580

[Image not found](#)

1-Octanol

Measured: 36.3

Predicted: 42.5

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1-Nonanol

Measured: 77.6

Predicted: 101

[Image not found](#)

Propylbenzene

Measured: 741

Predicted: 859

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1-Heptanol

Measured: 13.8

Predicted: 18.6